

Ab Initio Modeling of Point Defects and Gas Atoms in Beryllium

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Motivation

Beryllium is considered as the first wall armor material and as neutron multiplier for the blanket of fusion reactor. Radioactive hydrogen isotope T can be either implanted from plasma or generated through neutron induced nuclear reactions.

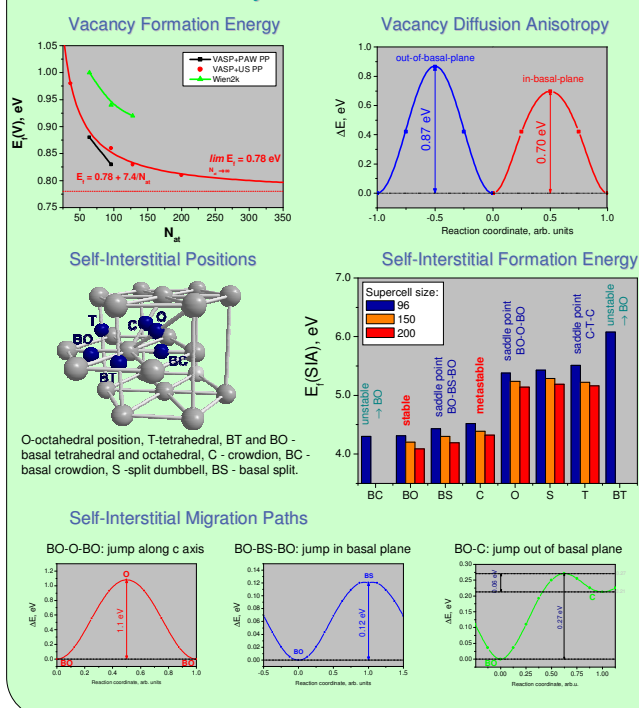
Retained tritium poses a potential safety and waste issue.

Modeling of tritium release from irradiated Be is indispensable for evaluation of the amount of retained T and extrapolation of the experimental results obtained using fission reactors to fusion irradiation conditions.

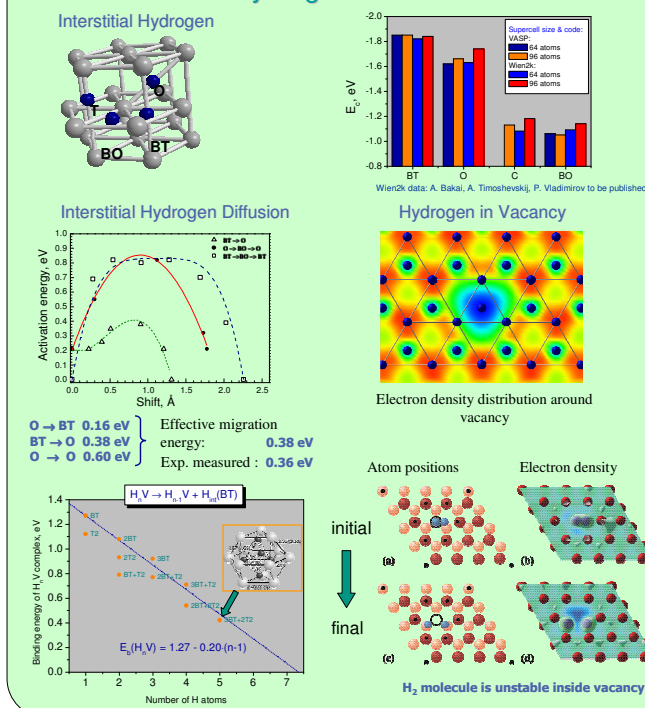
Simulation Method

- Density functional theory based code VASP
- generalized gradient approximation (GGA-PW91)
- Supercells: 64-200 atoms
- Convergence test of cut-off energy and the number of k-points
 - ENCUT = 450 eV
 - 13x13x13 k-points
- Diffusion barriers were calculated using nudged elastic band (NEB) method

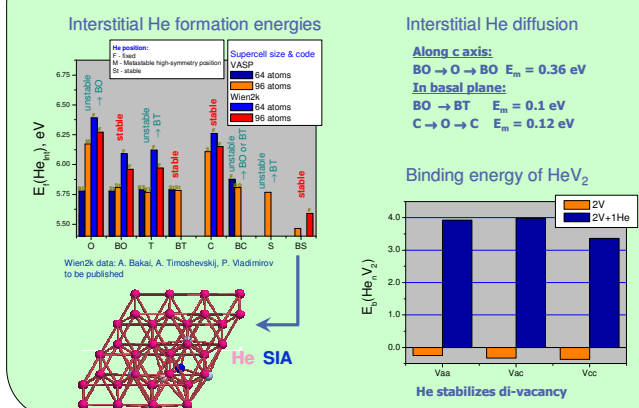
Vacancy and Self-Interstitials



Hydrogen in Be



He-Interstitials and He in Vacancies



Conclusions

- Di- and tri-vacancy clusters are unstable in Be, but are stabilized by gas atoms.
- DFT calculations correctly reproduce experimentally observed anisotropy of vacancy diffusion: 1.5 eV in basal and 1.67 eV out of basal plane.
- BO position is the most favorable for SIA in Be. C position is metastable. Other positions are unstable and usually represent saddle points along migration paths.
- SIA diffusion is anisotropic: 0.12 eV in basal plane and 0.27 eV out of it.
- BT position is the most favorable for the interstitial H. Effective migration energy is 0.38 eV in good agreement with exp. data (0.36 eV).
- Vacancy is an efficient trap for up to 5 H atoms: 0.4 - 1.27 eV.
- H₂ is unstable within a single vacancy. However, it is not excluded that it might be stable inside large vacancy clusters.
- Various He interstitial positions are stable: C, BO and BT, but the most favorable is basal split (BS) which relaxes to a kind of substitutional He - SIA cluster.
- Considered diffusion paths show anisotropic character of interstitial He diffusion: 0.1 eV in basal and 0.36 eV out of basal plane.

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